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"RIDGE ANALYSIS" OF RESPONSE SURFACES

by

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0. Introduction. In a 1959 paper, A. E. Hoerl discussed a method for examining a second order response surface. This paper provides a mathematically simpler derivation of the technique and proofs of some stated properties.

1. Lagrange's Undetermined Multipliers.

A well-known (e.g. Kaplan, 1956) method of obtaining the stationary or turning values of a function $f(x_1,x_2,\ldots,x_k)$ of k variables $x_1,x_2,\ldots, x_k$, subject to restrictions on the x_i such as

$$g_j(x_1,x_2,\ldots x_k) = 0, \qquad (j = 1,2,\ldots n)$$

is the following. Form the function

$$F = f - \sum_{j=1}^{n} \lambda_j g_j \tag{1.1}$$

where $\lambda_1, \lambda_2, \ldots \lambda_n$ are arbitrary. Differentiate (1.1) partially with respect to each x_i and set the results equal to zero. This will provide the k equations

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$$\frac{\partial F}{\partial x_i} \equiv \frac{\partial f}{\partial x_i} - \sum_{j=1}^{n} \lambda_j \frac{\partial g_j}{\partial x_i} = 0, \tag{1.2}$$

$$(i = 1,2,\ldots, k)$$

These k equations, with the additional n equations

$$g_j = 0 \quad , \qquad (j = 1, 2, \ldots, n) \tag{1.3}$$

provide $(n + k)$ equations which can be solved for the $(n + k)$ unknowns $x_1,x_2,\ldots,x_k$, $\lambda_1,\lambda_2,\ldots,\lambda_n$. Often the quantities λ_j are eliminated and not actually found; for this reason the words "undetermined multipliers" are used to describe them. In some cases, however, the solutions for $x_1,x_2,\ldots,x_k$ are easier to obtain if the λ_j are evaluated first; in other cases, as below, it may be easier to specify values of λ_j in equations (1.2) and regard other quantities in equations (1.3) as "undetermined", in their place.

Suppose, now that $(x_1,x_2,\ldots,x_k) = (a_1,a_2,\ldots,a_k)$ is a solution of equations (1.2) and (1.3) after elimination of λ_j.

Let $\underline{M}(\underline{x}) = \underline{M}(x_1,x_2,\ldots x_k) =$

$$\begin{bmatrix} \frac{\partial^2 F}{\partial x_1^2} & \frac{\partial^2 F}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 F}{\partial x_1 \partial x_k} \\ \frac{\partial^2 F}{\partial x_2 \partial x_1} & \frac{\partial^2 F}{\partial x_2^2} & \cdots & \frac{\partial^2 F}{\partial x_2 \partial x_k} \\ \cdots \\ \frac{\partial^2 F}{\partial x_k \partial x_1} & \frac{\partial^2 F}{\partial x_k \partial x_2} & \cdots & \frac{\partial^2 F}{\partial x_k^2} \end{bmatrix} \tag{1.4}$$

be the matrix of second order partial derivatives. Then if $\underline{M}(a_1,a_2,\ldots a_k) = \underline{M}(\underline{a})$, the resulting matrix after the solution $\underline{a}' = (a_1,a_2,\ldots a_k)$ has been substituted into (1.4) is

(a) positive definite, ie $\underline{y}'\ \underline{M}\ \underline{y} > 0$,

(b) negative definite, ie $\underline{y}'\ \underline{M}\ \underline{y} < 0$

where $\underline{y}' = (y_1,y_2,\ldots, y_k)$ is any 1 by k real vector, the function $f(x_1,x_2,\ldots,x_k)$ achieves

(a) a local minimum

(b) a local maximum.

respectively. For, if we expand F about $\underline{a}$ as a Taylor series of partial derivatives, remembering that all first partial derivatives of F are zero at $\underline{x} = \underline{a}$, we see that

$$F(\underline{a}+\underline{h}) - F(\underline{a}) = \tfrac{1}{2}\,\underline{h}'\ \underline{M}(\underline{a})\underline{h} + O(h^3)$$

where $\underline{h}$ represents a vector of small increments h_i all of the same order and $O(h^3)$ represents a remainder of third order in such increments. Thus, to order h^2, if $M(\underline{a})$ is positive definite,

$$F(\underline{a} + \underline{h}) > F(\underline{a}) \quad \text{, for } \underline{\text{all}} \text{ small } \underline{h}.$$

If $\underline{h}$ varies only in such a way that the restrictions are still satisfied, this implies that

$$f(\underline{a} + \underline{h}) > f(\underline{a})$$

ie, $f(\underline{a})$ is, locally, a minimum, subject to the restrictions holding. As we can see from this discussion, it might happen that

$$F(\underline{a} + \underline{h}) \not> F(\underline{a}) \text{ , for } \underline{\text{all}} \text{ small } \underline{h}$$

but

$$f(\underline{a} + \underline{h}) > f(\underline{a}) \text{ , for all } \underline{h} \text{ which satisfy the restrictions.}$$

Thus "$\underline{M}(\underline{a})$ is positive definite" is sufficient, but not necessary for a local restricted minimum of f at $\underline{x} = \underline{a}$. Similar remarks apply to the negative definite case. If $\underline{M}(\underline{a})$ is indefinite, further investigation of the function near the point $\underline{a}$ is required to determine what sort of stationary point has been obtained.

2. Improved derivation of the technique.

Consider the second order response surface in k variables $x_1, x_2, \ldots, x_k$, given by

$$\begin{aligned} \hat{y} = b_o + b_1x_1 + b_2x_2 + \ldots + b_kx_k \\ + b_{11}x_1^2 + b_{22}x_2^2 + \ldots + b_{kk}x_k^2 \\ + b_{12}x_1x_2 + \ldots + b_{k-1,k}\, x_{k-1}x_k . \end{aligned} \qquad (2.1)$$

The point $(0,0,\ldots,0)$ is the origin of measurement of the variables $x_1, x_2, \ldots x_k$. If the data used to obtain (2.1) resulted from a designed experiment, it would usually be the center of the design also. Suppose now we imagine a sphere, center at the origin $(0,0,\ldots,0)$ and of radius R, drawn in the x-space.

Then at some points on the sphere there will be a maximum $\hat{y}$ and elsewhere a minimum $\hat{y}$, and possibly also (depending on the type of quadratic surface (2.1) obtained and the value of R) values of $\hat{y}$ which are local maxima or minima, that is, maxima or minima for all nearby points on the sphere, but not absolute maxima and minima when all points of the sphere are taken into consideration. If we investigate the stationary values of the function $\hat{y}$ on the sphere, ie the stationary values subject to the restriction

$$g(x_1, x_2, \ldots, x_k) \equiv x_1^2 + x_2^2 + \ldots + x_k^2 - R^2 = 0, \quad (2.2)$$

we shall be able to find all these local and absolute maxima and minima.

We can then plot against R as abscissa the following (k+1) ordinates: $x_1, x_2, \ldots, x_k$, $\hat{y}$ for, say, the absolute maximum of $\hat{y}$ found on the sphere radius R.

If we change R slightly the appropriate values of $x_1, x_2, \ldots,$ x_k and $\hat{y}$ for the absolute maximum will also change slightly and so, by varying R, we can construct (k+1) curves showing how the position and magnitude of the absolute maximum $\hat{y}$ change as R changes. We can thus find, for any selected R, the place of maximum yield on the response surface. Such a plot can also be made of absolute minimum or of the loci of intermediate stationary values, as desired. Mathematically, then, we wish to find the stationary values of $\hat{y} = f(x_1, x_2, \ldots x_k)$, from equation (2.1), subject to the restriction $g(x_1, x_2, \ldots, x_k) = 0$ as in equation (2.2).

Using the method of Lagrange multipliers we set $F = \hat{y} - \lambda g$ and equations (1.2) after rearrangement and division by a factor of 2 become*

$$\begin{aligned}
(b_{11} - \lambda)\, x_1 + \tfrac{1}{2}b_{12}x_2 + \ldots \quad &+ \tfrac{1}{2}b_{1k}x_k = -\tfrac{1}{2}b_1 \\
\tfrac{1}{2}b_{12}x_1 + (b_{22} - \lambda)x_2 + \ldots \quad &+ \tfrac{1}{2}b_{2k}x_k = -\tfrac{1}{2}b_2 \\
\cdots\cdots \quad & \\
\tfrac{1}{2}b_{1k}x_1 + \tfrac{1}{2}b_{2k} + \ldots \quad &+ (b_{kk} - \lambda)x_k = -\tfrac{1}{2}b_k
\end{aligned} \qquad (2.3)$$

or in matrix notation

$$(\underline{B} - \lambda\, \underline{I})\underline{x} = -\tfrac{1}{2}\underline{b} \qquad (2.4)$$

where

$$\underline{B} = \begin{bmatrix} b_{11} & \tfrac{1}{2}b_{12} & \ldots & \tfrac{1}{2}b_{1k} \\ \tfrac{1}{2}b_{12} & b_{22} & \ldots & \tfrac{1}{2}b_{2k} \\ ----- & & & \\ \tfrac{1}{2}b_{1k} & \tfrac{1}{2}b_{2k} & \ldots & b_{kk} \end{bmatrix}, \quad \underline{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \end{bmatrix} \qquad (2.5)$$

and $\underline{I}$ is the k by k unit matrix.

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*Note: If we set $k=3$ and $\alpha = 2(\lambda - b_{33})$, ie $\lambda = \tfrac{1}{2}\alpha + b_{33}$, we reduce to the unsymmetrical equations obtained by Hoerl with α as parameter.

Then, theoretically, the (k+1) equations (2.4) and (2.2) can be solved for sets of $x_1, x_2, \ldots x_k$, and λ corresponding to the various stationary values of $\hat{y}$ on the sphere radius R. Since the solution in this form leads to involved calculations, a simpler and equivalent method of solution may be used as follows.

(1) Regard R as variable, but fix λ instead.

(2) Insert the selected value of λ in equations (2.4) and solve them for $x_1, x_2, \ldots x_k$. The solution is used in steps 3and 4.

(3) Compute $R = (x_1^2+x_2^2+\ldots+x_k^2)^{\frac{1}{2}} = (\underline{x}'\underline{x})^{\frac{1}{2}}$, where $\underline{x}' = (x_1, x_2, \ldots, x_k)$

(4) Evaluate $\hat{y}$.

We now have a set of numbers $(\lambda, x_1, x_2, \ldots, x_k, R, \hat{y})$ and know that on the sphere radius R, center the origin there is a stationary value of $\hat{y}$, value determined, at the point $(x_1, x_2, \ldots, x_k)$. Several different values of λ will give rise to several stationary points which lie on the same sphere radius R. Whether a particular stationary value is the absolute maximum, absolute minimum, a local maximum or a local minimum is determined, as we shall see, by the value of λ.

3. Properties of the stationary values.

Let the eigen values or latent roots of the matrix $\underline{B}$ be denoted by μ_i $(i = 1, 2, \ldots k)$. Then the μ_i are such that

$$\underline{B}\ \underline{x} = \mu\ \underline{x}, \tag{3.1}$$

or

$$(\underline{B} - \mu\ \underline{I})\ \underline{x} = \underline{0}. \tag{3.2}$$

Hence

$$\det\ (\underline{B} - \mu\ \underline{I}) = 0, \tag{3.3}$$

where "det" denotes "the determinant of", provides a kth degree equation with roots $\mu_1, \mu_2, \ldots \mu_k$, say. Note that when a standard canonical reduction is made of equation (2.1), $\mu_1, \mu_2, \ldots, \mu_k$ are the latent roots needed to reduce $\hat{y}$ to the form

$$\hat{y} = y_0 + \mu_1 X_1^{\,2} + \mu_2 X_2^{\,2} + \ldots + \mu_k X_k^{\,2}.$$

Canonical reduction is another way of examining a second order response surface for its main features (C. L. Davies, 1956). By comparing the value λ, which corresponds to any particular stationary value of $\hat{y}$ on a sphere of radius R, with the latent roots μ_i we shall be able to determine what sort of stationary value has been obtained.

Suppose $\lambda = \lambda_1$ and $\lambda = \lambda_2$ are substituted in equation (2.4) and the solutions $\underline{x}_1' = (a_1, a_2, \ldots, a_k)$ and $\underline{x}_2' = (c_1, c_2, \ldots c_k)$ result, thus providing two stationary values $\hat{y}_1$ and $\hat{y}_2$ of $\hat{y}$ on the spheres $\underline{x}'\underline{x} = R_1^2$ and $\underline{x}'\underline{x} = R_2^2$, respectively. Then the following results are true.

<u>Result 3.1</u>: If $R_1 = R_2$ and $\lambda_1 > \lambda_2$, the $\hat{y}_1 > \hat{y}_2$.

<u>Proof</u>: We know that

$$(\underline{B} - \lambda_1\ \underline{I})\ \underline{x}_1 = -\tfrac{1}{2}\underline{b}\ , \tag{3.1.1}$$

$$(\underline{B} - \lambda_2\ \underline{I})\ \underline{x}_2 = -\tfrac{1}{2}\underline{b}\ , \tag{3.1.2}$$

$$\underline{x}_1'\underline{x}_1 = \underline{x}_2'\,\underline{x}_2 = R^2 \text{ , say,} \tag{3.1.3}$$

$$\hat{y}_1 = \underline{x}_1'\,\underline{B}\,\underline{x}_1 + \underline{x}_1'\,\underline{b} + b_o \text{ ,} \tag{3.1.4}$$

and
$$\hat{y}_2 = \underline{x}_2'\,\underline{B}\,\underline{x}_2 + \underline{x}_2'\,\underline{b} + b_o . \tag{3.1.5}$$

Premultiplying (3.1.1) and (3.1.2) by $\underline{x}_1'$ and $\underline{x}_2'$ respectively and subtracting, and remembering (3.1.3), gives

$$\underline{x}_1'\underline{B}\,\underline{x}_1 - \underline{x}_2'\underline{B}\,\underline{x}_2 + \tfrac{1}{2}(\underline{x}_1 - \underline{x}_2)'\,\underline{b} = (\lambda_1 - \lambda_2)\,R^2 \text{ ,} \tag{3.1.6}$$

whence, using (3.1.4) and (3.1.5),

$$\hat{y}_1 - \hat{y}_2 = \tfrac{1}{2}(\underline{x}_1 - \underline{x}_2)'\,\underline{b} + (\lambda_1 - \lambda_2)\,R^2 \tag{3.1.7}$$

Premultiplying (3.1.1) and (3.1.2) by x_2' and $\underline{x}_1'$ respectively and subtracting gives

$$(\lambda_2 - \lambda_1)\,\underline{x}_1'\underline{x}_2 = \tfrac{1}{2}(\underline{x}_1 - \underline{x}_2)'\,\underline{b} \tag{3.1.8}$$

since $\underline{x}_2'\,\underline{B}\,\underline{x}_1 = \underline{x}_1'\,\underline{B}\,\underline{x}_2$ and $\underline{x}_2'\underline{x}_1 = \underline{x}_1'\underline{x}_2$. Hence from (3.1.7) and (3.1.8)

$$\hat{y}_1 - \hat{y}_2 = (\lambda_1 - \lambda_2)\,(R^2 - \underline{x}_2'\underline{x}_1) \tag{3.1.9}$$

But $R^2 - \underline{x}_2'\underline{x}_1 = (a_1^2 + a_2^2 + \ldots + a_k^2)^{\frac{1}{2}}(c_1^2 + c_2^2 + \ldots + c_k^2)^{\frac{1}{2}}$

$- (a_1c_1 + a_2c_2 + \ldots + a_kc_k) > 0$, always, by a well-known inequality (Hardy, Littlewood and Polya, 1952).

Hence $\lambda_1 > \lambda_2$ **implies** $\hat{y}_1 > \hat{y}_2$.

<u>Result 3.2</u>: If $R_1 = R_2$, $\underline{M}(\underline{x}_1)$ **is** positive definite and $\underline{M}(\underline{x}_2)$ is indefinite, then $\hat{y}_1 < \hat{y}_2$.

<u>Proof</u>: By hypothesis

$\underline{y}'(\underline{B} - \lambda_2\,\underline{I})\,\underline{y} \le 0$, for at least one $\underline{y} = q$, say

$y'(B - \lambda_1\,I)\,y > 0$, for all $\underline{y}$, including $\underline{y} = \underline{q}$.

Hence $$\lambda_2 \underline{q}'\underline{q} \geq \underline{q}' \underline{B} \underline{q} > \lambda_1 \underline{q}'\underline{q}$$

which implies $$\lambda_2 > \lambda_1.$$

By Result 3.1 then, $\hat{y}_1 < \hat{y}_2$.

Similarly, if $R_1 = R_2$, $\underline{M}(\underline{x}_1)$ is negative definite and $\underline{M}(\underline{x}_2)$ is indefinite, then $\hat{y}_1 > \hat{y}_2$.

Result 3.3: If $\lambda_1 > \mu_i$ (all i), then $\underline{x}_1$ is a point at which $\hat{y}$ attains a local maximum on the sphere radius R_1; if $\lambda_1 < \mu_i$ (all i), then $\underline{x}_1$ is a point at which $\hat{y}$ attains a local minimum on the sphere radius R_1. (As will be seen later, we obtain the absolute maximum and minimum in this way, not only the local maximum and minimum.)

Proof: It will be seen that equation (1.4) becomes

$$M(\underline{x}_1) = \underline{B} - \lambda_1 \underline{I}$$

for the stationary point $\underline{x}_1$. Then if $\underline{y}$ is any n by 1 vector, the quadratic form

$$\begin{aligned} \underline{y}' \underline{M}(\underline{x}_1) \underline{y} &= \underline{y}'(\underline{B} - \lambda_1 \underline{I}) \underline{y} \\ &= \underline{y}' \underline{By} - \lambda_1 \underline{y}'\underline{y} \\ &= \underline{y}'\underline{y} (\mu - \lambda_1) \end{aligned}$$

if μ is any latent root of B.

Thus, if $\lambda_1 > \mu_i$, (all i), $\underline{M}(\underline{x}_1)$ is negative definite and hence $\underline{x}_1$ is a point on the sphere radius R at which $\hat{y}$ attains a maximum, if $\lambda_1 < \mu_i$ all i, $\underline{M}(\underline{x}_1)$ is positive definite and hence $\underline{x}_1$ is a point on the sphere, radius R at which $\hat{y}$ attains a minimum.

Result 3.4: Suppose, as R increases, we trace a locus of stationary points (the absolute maximum, absolute minimum, or a local maximum or minimum) and examine the changing values of $\hat{y}$. Then, as R increases, $\hat{y}$ changes in one of the following ways (when the response surface is quadratic):

(a) decreases monotonically

(b) increases monotonically

(c) passes through a maximum and then decreases monotonically

(d) passes through a minimum and then increases monotonically

If (c) and (d) happen, it is because the locus has passed through the center of the quadratic system.

Proof:
$$\hat{y} = b_0 + \underline{x}'\underline{B}\,\underline{x} + \underline{x}'\,\underline{b}$$
$$= b_0 + \lambda\,\underline{x}'\underline{x} + \tfrac{1}{2}\underline{x}'\underline{b}\ , \tag{3.4.1}$$

using equation (2.4).

Suppose we make a small change $\delta\lambda$ in λ; this will induce small changes $\delta\underline{x}$ in $\underline{x}$, in equations (2.4), a small change δR in R and finally a small change $\delta\hat{y}$ in $\hat{y}$. Then, from (3.4.1),

$$\hat{y} + \delta\hat{y} = b_0 + (\lambda + \delta\lambda)\ (\underline{x} + \delta\underline{x})'\ (\underline{x} + \delta\underline{x}) + \tfrac{1}{2}(\underline{x} + \delta\underline{x})'\underline{b} \tag{3.4.2}$$

Subtracting (3.4.1) from (3.4.2) and rearranging the result, we find

$$\delta\hat{y} = 2\lambda\,\underline{x}'\delta\underline{x} + \delta\lambda\,\underline{x}'\underline{x} + \tfrac{1}{2}\,\delta\underline{x}'\underline{b} + Q_2 \tag{3.4.3}$$

where Q_2 denotes terms of second order in $\delta\lambda$ and $\delta\underline{x}$.

But if we set $\lambda_2 = \lambda + \delta\lambda$, $\lambda_1 = \lambda$, $\underline{x}_2 = \underline{x} + \delta\underline{x}$ and $\underline{x}_1 = \underline{x}$ in equation (3.4.8), we see that

$$\delta\lambda\underline{x}'\underline{x} + \tfrac{1}{2}\delta\underline{x}'\underline{b} = Q_2' \qquad (3.4.4)$$

where Q_2' denotes (other) terms of second order in $\delta\lambda$ and $\delta\underline{x}$.

Thus (3.4.3) and (3.4.4) imply that

$$\delta\hat{y} = 2\,\lambda\,\underline{x}'\delta\underline{x} + Q_2'' \qquad (3.4.5)$$

ie $$\delta\hat{y} = 2\,\lambda\,R\delta R + Q_2'', \qquad (3.4.6)$$

since $\underline{x}'\underline{x} = R^2$. Dividing by δR and letting all increments tend to zero gives

$$\frac{\partial y}{\partial R} = 2\,\lambda\,R \qquad (3.4.7)$$

which is zero when $R = 0$ and when $\lambda = 0$. When $R = 0$ we are at the origin and the value of $\hat{y}$ when $R = 0$ is the starting value for the locus of absolute maximum and absolute minimum $\hat{y}$. When $R \neq 0$, $\hat{y}$ is stationary with respect to R only when $\lambda = 0$, but if $\lambda = 0$, equations (2.4) yield, as solution, the center of the second order surface, since we shall obtain the point at which

$$\frac{\partial\hat{y}}{\partial x_i} = 0. \qquad (i = 1,2,\ldots,k) \qquad (3.3.8)$$

The stated result follows. Any locus passing through the center of the surface satisfies (c) or (d). Otherwise it satisfies (a) or (b).

4. Comments

Hoerl (1959) states similar but not quite identical properties and ascribes their proof to Dr. R. Jackson of the University of Delaware. No proof, nor any reference, is given in the paper however.

The four results have the following implication. If we wish to follow a locus of the absolute maximum $\hat{y}$ for increasing R, we should substitute in equation (2.4) only values of λ greater than all the latent roots of $\underline{B}$. This will make $\underline{M}(\underline{x})$ negative definite and will ensure that $\hat{y}$ is a local maximum for every solution $\underline{x}$. (It is in fact an absolute maximum as we shall soon see.) No value of λ less than the greatest latent root should be considered in such a case for, while values of λ between eigen values may provide a local maximum or minimum they cannot provide an <u>absolute</u> maximum or minimum.

In fact the total range of λ, namely $-\infty$ to ∞ is divided into sections by the latent roots $\mu_1, \mu_2, \ldots, \mu_k$. Suppose $\mu_1 \leqslant \mu_2 < \ldots < \mu_k$. Then we have (k+1) intervals $(-\infty, \mu_1)$, (μ_1, μ_2), ... (μ_{k-1}, μ_k) (μ_k, ∞).

As $\lambda \rightarrow \mu_i$ (i=1,2,...,k), the resulting solution $\underline{x} \rightarrow \pm \infty$ so that $R \rightarrow \infty$. As $\lambda \rightarrow \pm \infty$, $\underline{x} \rightarrow \underline{0}$ and so $R \rightarrow 0$. Furthermore the value of $\frac{\partial^2 R}{\partial \lambda^2}$ is positive for all $R \neq 0$.and is zero when $R = 0$. For we know that

$$(\underline{B} - \lambda\ \underline{I})\ \underline{x} = -\tfrac{1}{2}\underline{b} \qquad (4.1)$$

$$\underline{x}'\underline{x} = R^2 \qquad (4.2)$$

Differentiating once with respect to λ gives

$$(\underline{B} - \lambda\ \underline{I}) \frac{\partial \underline{x}}{\partial \lambda} = \underline{x}, \qquad (4.3)$$

and

$$\underline{x}' \frac{\partial \underline{x}}{\partial \lambda} = R \frac{\partial R}{\partial \lambda} \qquad (4.4)$$

A second differentiation with respect to λ gives

$$(\underline{B} - \lambda\ \underline{I}) \frac{\partial^2 \underline{x}}{\partial \lambda^2} = 2 \frac{\partial \underline{x}}{\partial \lambda} \qquad (4.5)$$

and

$$\underline{x}' \frac{\partial^2 \underline{x}}{\partial \lambda^2} + \frac{\partial \underline{x}'}{\partial \lambda} \frac{\partial \underline{x}}{\partial \lambda} = R \frac{\partial^2 R}{\partial \lambda^2} + \left(\frac{\partial R}{\partial \lambda}\right)^2 \qquad (4.6)$$

If we premultiply (4.3) and (4.5) by $\frac{\partial^2 \underline{x}'}{\partial \lambda^2}$ and $\frac{\partial \underline{x}'}{\partial \lambda}$ respectively, subtract, and transpose, we find

$$\underline{x}' \frac{\partial^2 \underline{x}}{\partial \lambda^2} - 2 \frac{\partial \underline{x}'}{\partial \lambda} \frac{\partial \underline{x}}{\partial \lambda} = 0. \qquad (4.7)$$

This, substituted in (4.6), leads to

$$R \frac{\partial^2 R}{\partial \lambda^2} = 3 \frac{\partial \underline{x}'}{\partial \lambda} \frac{\partial \underline{x}}{\partial \lambda} - \left(\frac{\partial R}{\partial \lambda}\right)^2 \qquad (4.8)$$

Now

$$\frac{\partial R}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left\{\underline{x}'\underline{x}\right\}^{\frac{1}{2}} = \underline{x}' \frac{\partial \underline{x}}{\partial \lambda} \Big/ (\underline{x}'\underline{x})^{\frac{1}{2}} \qquad (4.9)$$

Thus, using (4.9) in (4.8),

$$R^3 \frac{\partial^2 R}{\partial \lambda^2} = 2R^2 \frac{\partial \underline{x}'}{\partial \lambda} \frac{\partial \underline{x}}{\partial \lambda} + \left\{\underline{x}'\underline{x} \frac{\partial \underline{x}'}{\partial \lambda} \frac{\partial \underline{x}}{\partial \lambda} - \left(\underline{x}' \frac{\partial \underline{x}}{\partial \lambda}\right)^2\right\} \qquad (4.10)$$

The first part of the right member of (4.10) is always non-negative and is zero only when R=0 or when $\frac{\partial x}{\partial \lambda} = 0$. The second part of the right member of (4.10) is always non-negative by a well-known inequality (Hardy, Littlewood and Polya, 1952) and is zero only when $\underline{x} = \underline{0}$, ie R = 0, or when $\frac{\partial x}{\partial \lambda} = 0$. When $\frac{\partial x}{\partial \lambda} = 0$, $\underline{x} = \underline{0}$ by (4.3) if $\lambda \neq \mu_i$, and thus R = 0. Thus $\frac{\partial^2 R}{\partial \lambda^2}$ is positive except when R = 0, when it takes the value zero.

Note that $\frac{\partial R}{\partial \lambda} = 0$ does <u>not</u> imply that $\frac{\partial x}{\partial \lambda} = 0$ (and so that $\underline{x} = 0$ and R = 0) because the left member of (4.4) can be zero due to the cancellation of positive and negative cross-products.

From the above, we see that the graph of R, plotted as ordinate against λ as abscissa, acts as follows.

At $\lambda = -\infty$, R = 0 and R increases steadily to infinity at $\lambda = \mu_1$; between pairs of latent roots, R passes down from infinity at μ_i through a stationary value and up to infinity again at μ_{i+1}. Finally R passes from infinity at μ_k to zero at $\lambda = \infty$. (See Figure 1).

Suppose we consider what happens for various values of R. Each value of R can give rise to, at most, 2k corresponding values of λ. The number will be less if some of the loops in Figure 1 have their lowest point above the value of R being considered. It is clear too, that if we wish to find the locus of the absolute minimum of $\hat{y}$ as R varies we can substitute any values of λ less than the smallest latent root μ_1 into (2.4) and obtain a point on the locus, since there is only one such locus and thus there can be no ambiguity. A similar remark is true for the locus of the absolute maximum $\hat{y}$ as R varies. When we choose values of λ between latent roots, however, we may be on either of two loci of stationary values , depending on whether we are to the right or left of the value of λ for which R is stationary.

As indicated above, not all of the loci appear for every value of R, but as R increases, more and more appear. Since the fitted model can be considered accurate only within the region of the experimental design, loci which do not appear except for large R are usually of little interest.

To summarize the main practical feature of this work: Suppose we wish to follow the absolute maximum predicted value of $\hat{y}$ on a sphere of radius R, as R increases. Find the latent roots of $\underline{B}$, choose values of λ greater then all of these roots and substitute them into (2.4). Solve for $\underline{x}$, evaluate $R^2 = \underline{x}'\underline{x}$ and $\hat{y}$ and plot $\hat{y}, x_1, x_2, \ldots, x_k$ against R. (Similar work, choosing values of λ less then all of the latent roots of $\underline{B}$, can be carried out for an investigation of the absolute minimum value of $\hat{y}$ on spheres of radius R).

5. Example:

This example was used by Hoerl. Consider the response surface in two factors

$$\hat{y} = 80 + 0.1x_1 + 0.2x_2 + 0.2x_1^2 + 0.1x_2^2 + x_1x_2 \qquad (5.1)$$

Thus

$$\underline{B} = \begin{bmatrix} 0.2 & 0.5 \\ 0.5 & 0.1 \end{bmatrix} \quad \underline{b} = \begin{bmatrix} 0.1 \\ 0.2 \end{bmatrix} \qquad (5.2)$$

Equations (2.4) become

$$\begin{aligned} (0.2 - \lambda)x_1 + 0.5x_2 &= -0.05, \\ 0.5x_1 + (0.1-\lambda)x_2 &= -0.10, \end{aligned} \qquad (5.3)$$

with solution

$$\begin{aligned} x_1 &= (9 + 10\lambda) / 2D \\ x_2 &= (1 + 20\lambda) / 2D \end{aligned} \qquad (5.4)$$

where

$$D = 100 \det(\underline{B} - \lambda \underline{I}) = 100\lambda^2 - 30\lambda - 23 \qquad (5.5)$$

The eigen values or latent roots of $\underline{B}$ are given by $D = 0$, whence

$$\lambda = 0.652 \text{ or } -0.352. \qquad (5.6)$$

(Note: Hoerl's parameter, which we shall call α, is such that $\lambda = b_{22} + \frac{1}{2}\alpha$, ie $\alpha = 2(\lambda - 0.1)$ for the example. This will lead to his corresponding eigen values of $\alpha = 1.105$ and -0.905, apart from rounding **error.** Note that when $\lambda = 0.2$, $\alpha = 0.2$. In general putting λ and α equal to the same number would produce different stationary points in the two calculations and the fact that our calculation below with $\lambda = 0.2$ produces the <u>same</u> stationary point as Hoerl should have obtained with $\alpha = 0.2$ is pure coincidence due to the numbers involved.)

If now we wish to look for the locus of the absolute minimum (or maximum) of $\hat{y}$ on circles $x_1^2 + x_2^2 = R^2$ of radius R, we should insert in equations (5.4) values of λ less (or greater) than both eigen values (5.6), ie $\lambda < -0.352$ (or $\lambda > 0.652$).

Suppose we select a value $\lambda = 0.2$. Then equations (5.4) and (5.5) yield solution $(x_1, x_2) = (-0.22, -0.10)$; there is a calculation error here in Hoerl's paper. Then $R = 0.242$, so that on the circle $x_1^2 + x_2^2 = 0.242$, $\hat{y}$ is stationary at the point (-0.22, -0.10) but, since $-0.352 < \lambda = 0.2 < 0.652$, this stationary value $\hat{y} = 79.99$ is neither an absolute maximum or minimum.

Continued substitution of values of λ into equations (5.4) and (5.5) will yield four loci of stationary values as R increases and these, as evaluated by Hoerl, are shown in Figure 2.

The loci of absolute maximum and absolute minimum, curves 1 and 4, begin at R = 0 and correspond to values of λ beginning at $\lambda = \infty$ and $\lambda = -\infty$, respectively. The two loci of intermediate stationary values do not begin until R = 0.195 and correspond to $\lambda = -0.003$, when $\frac{\partial R}{\partial \lambda} = 0$, ie we are at the bottom of the loop of R, plotted against λ, which lies between the latent roots $\mu_1 = -0.352$ and $\mu_2 = 0.652$. Because of the scale of the diagram, the difference in starting points cannot be distinguished.

The response surface given by equation (4.1) is in fact a saddle, rising in the first and third quadrants of the (x_1, x_2)

plane, falling in the second and fourth quadrants, with ridges oriented approximately 45^{o} to the axes and with center slightly off the origin at (- 9/46, - 1/46). Thus the locus of absolute maxima in Figure 2 passes from the origin out the first quadrant of the (x_1,x_2) plane, the locus of absolute minima passes out the fourth quadrant and the other two loci of stationary points, which are loci of neither absolute maxima or absolute minima, pass out the second and third quadrants.

Figure I THE DEPENDENCE OF R ON λ

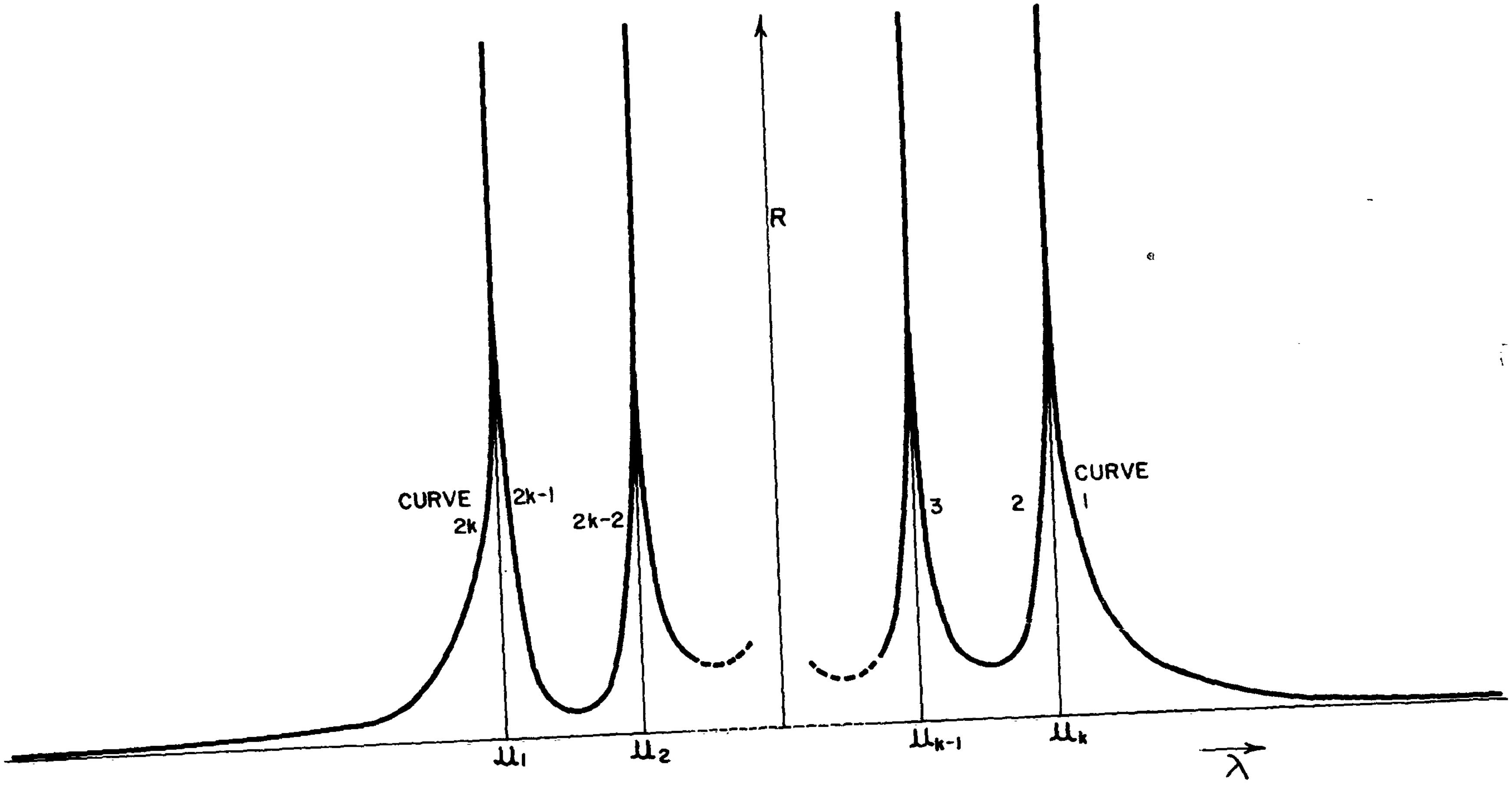
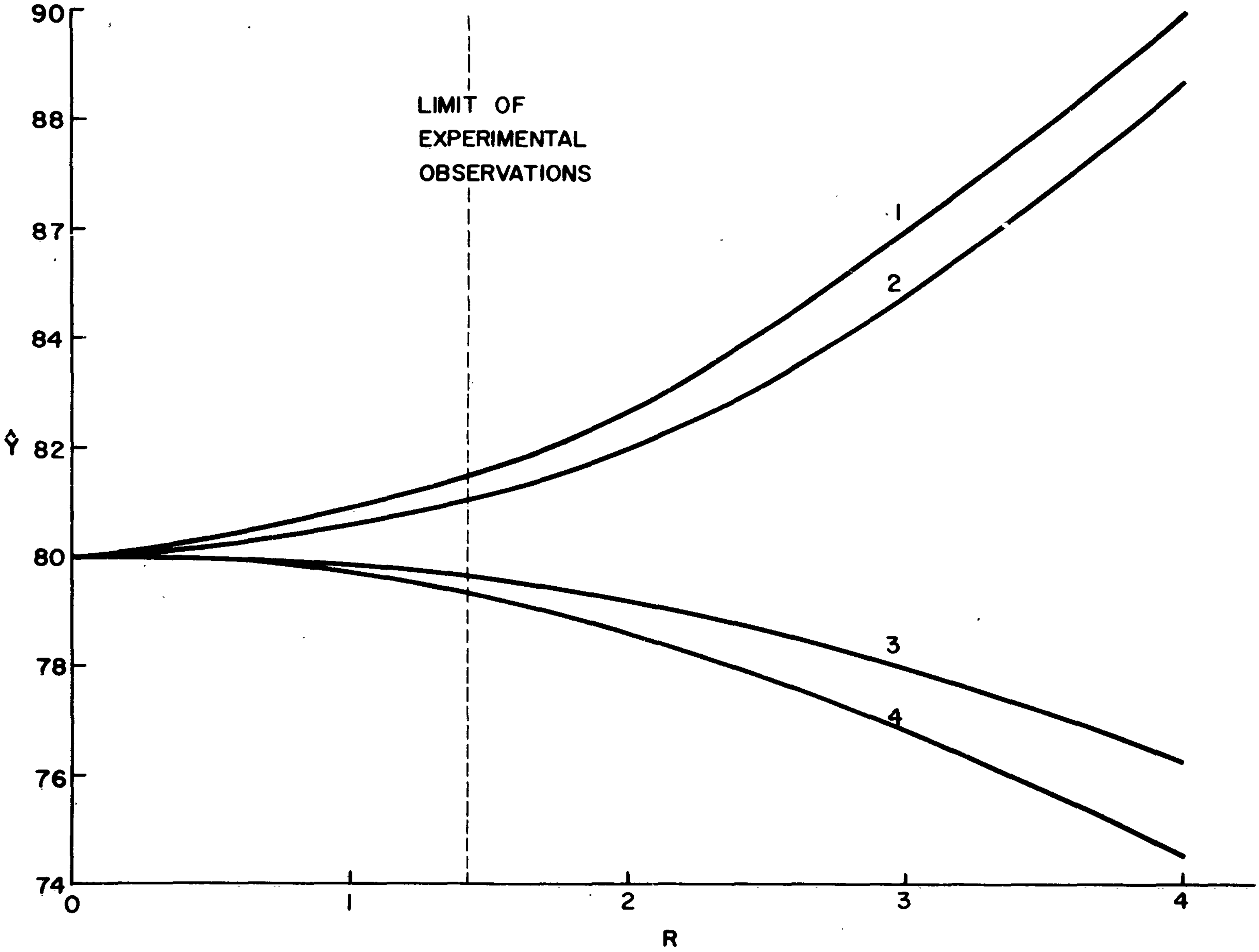


Figure 2 LOCI OF STATIONARY VALUES AS R VARIES



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